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STRUCTURE FILE UPDATES:     7 NOV 2006  HIGHEST RN 912617-52-8
DICTIONARY FILE UPDATES:    7 NOV 2006  HIGHEST RN 912617-52-8

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on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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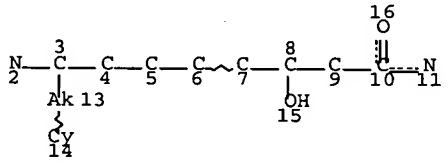

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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STEREO ATTRIBUTES: NONE
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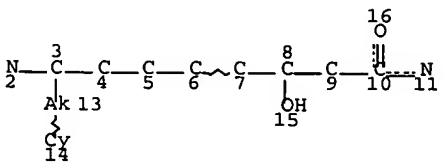

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STEREO ATTRIBUTES: NONE
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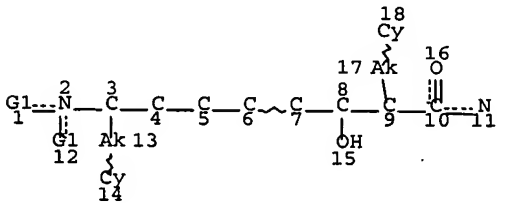

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STEREO ATTRIBUTES: NONE
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FILE COVERS 1907 - 8 Nov 2006 VOL 145 ISS 20
FILE LAST UPDATED: 7 Nov 2006 (20061107/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d bib abs hitrn fhitstr retable l21 tot

L21 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:333687 HCAPLUS Full-text
DN 140:339637
TI Preparation of peptidomimetic μ-opioid receptor ligands
IN **Harrison, Bryce; Gierasch, Tiffany Malinky; Verdine, Gregory L.; Shi, Zhangjie**
PA President and Fellows of **Harvard** College, USA
SO PCT Int. Appl., 128 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO2004033414	A1	20040422	2003WO-US32280	20031010
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU2003279953	A1	20040504	2003AU-0279953	20031010
US2004254225	A1	20041216	2003US-0683756	20031010
PRAI 2002US-417925P	P	20021011		
2003US-443428P	P	20030129		
2003WO-US32280	W	20031010		

OS MARPAT 140:339637
AB The invention relates to peptidomimetic compds. derived from aralkyl-substituted aminodihydroxyalk(en)oic acids which are modulators of the μ-opioid receptor (MOR) and thus have therapeutic applications. The claims include compds. of general formula R52NCHR1CH(OH)CH2CHRCHRCH(OH)CHR2CO-X-CHR3R4 [R2 is H2 or a bond; X is N, O or S; R1-R3 are (un)substituted (hetero)arylalkyl; R4 is H, CONR72 (R7 is H, alkyl, acyl or a protecting group), CONHR7, CH2OH, CH(OH)CH:CH2 or CONHCHR10CO2H (R10 is an amino acid side chain); R5 is H, alk(en)yl, (hetero)aryl, acyl, a protecting group or COCHR10CO2H] or their pharmaceutically-acceptable salts. Thus, stereoisomeric H2NCH(CH2C6H4OH-p)CH(OH)CH2CH:CHCH(OH)CH(CH2Ph)CONHCH(CH2Ph)CONH2 (2) were prepared and assayed for binding affinity for MOR [8.8 ± 0.7 nM for (S,S,S,R)-2, vs. 1.2 ± 0.1 nM for endomorphin 2].
IT **479495-67-5P 479495-68-6P 479495-69-7P**
479495-70-0P 479495-71-1P 479495-72-2P
479495-73-3P 479495-74-4P 479495-75-5P
479495-76-6P 479495-77-7P 479495-78-8P
479495-79-9P 479495-80-2P 479495-81-3P
479495-83-5P 479495-84-6P 479495-85-7P
479495-86-8P 479496-03-2P 479496-04-3P
479496-05-4P 479496-06-5P 479496-11-2P
479496-12-3P 479496-13-4P 479496-14-5P
479496-15-6P 479496-16-7P 479496-17-8P
479496-18-9P 479496-19-0P 503186-38-7P
503186-39-8P 503186-40-1P 503186-41-2P
503186-42-3P 503186-43-4P 503186-44-5P
503186-45-6P 503186-46-7P 503186-47-8P
503186-48-9P 507276-41-7P 507276-43-9P
507276-45-1P 507276-47-3P 507276-49-5P
507276-51-9P 507276-53-1P 507276-55-3P
507276-57-5P 507276-59-7P 507276-61-1P
507276-63-3P 507276-65-5P 507276-67-7P
507276-69-9P 507276-71-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidomimetic μ-opioid receptor ligands)
IT **680187-48-8DP**, resin-bound **680187-49-9DP**, resin-bound

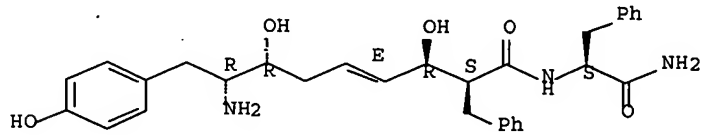
680187-50-2DP, resin-bound **680187-51-3DP**, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidomimetic μ-opioid receptor ligands)

IT **479495-67-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidomimetic μ-opioid receptor ligands)

RN 479495-67-5 HCAPLUS

CN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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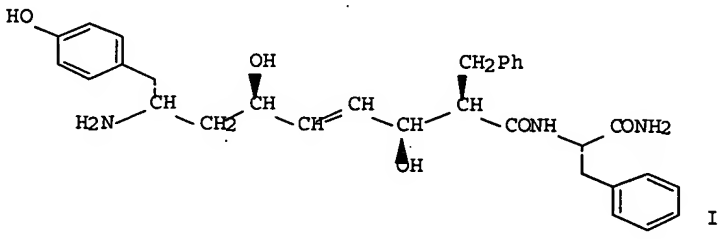
Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Gierasch	2000	2	3999	ORGANIC LETTERS	HCAPLUS
Harrison, B	2002	124	13352	J AM CHEM SOC	HCAPLUS
Harrison, B	2003	46	677	J MED CHEM	HCAPLUS
Sepracor Inc	1999			WO---9965932 A	HCAPLUS

L21 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:110339 HCAPLUS Full-text
DN 138:297095
TI Unpredictable Stereochemical Preferences for Mu Opioid Receptor Activity in an Exhaustively Stereodiversified Library of 1,4-Enediols
AU **Shi, Zhangjie; Harrison, Bryce A.; Verdine, Gregory L.**
CS Department of Chemistry and Chemical Biology, **Harvard** University, Cambridge, MA, 02138, USA
SO Organic Letters (2003), 5(5), 633-636
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 138:297095
GI



I

AB Using olefin cross-metathesis, the authors synthesized a novel stereodiversified library of I containing a trans-1,4-enediol. Screening this library for mu opioid receptor (MOR) affinity identified multiple high-affinity ligands and revealed that the stereochem. configuration varied widely among those ligands having the highest affinity. It was not possible to predict the configurations of the most active I stereoisomers on the basis of the configuration of endomorphin-2, a known MOR peptide ligand, validating the diversity-based approach to ligand discovery.

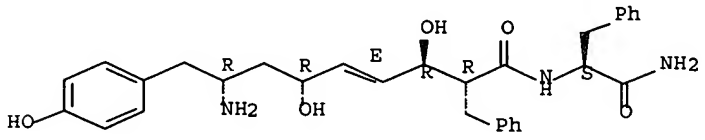
IT **507276-41-7P 507276-43-9P 507276-45-1P**
507276-47-3P 507276-49-5P 507276-51-9P
507276-53-1P 507276-55-3P 507276-57-5P
507276-59-7P 507276-61-1P 507276-63-3P
507276-65-5P 507276-67-7P 507276-69-9P
507276-71-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(unpredictable stereochem. preferences for mu opioid receptor activity in an exhaustively stereodiversified library of enediols in relation to partial agonist activity)

IT **507276-41-7P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(unpredictable stereochem. preferences for mu opioid receptor activity in an exhaustively stereodiversified library of enediols in relation to partial agonist activity)

RN 507276-41-7 HCAPLUS

CN Benzenepropanamide, α-[(1R,2E,4R,6R)-6-amino-1,4-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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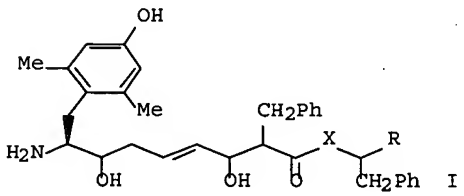
Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Blackwell, H	2000	122	58	J Am Chem Soc	HCAPLUS
Bylund, D	1990		1	Methods in Neurotran	
Dooley, C	1999	51	379	Biopolymers	HCAPLUS
Furstner, A	2000	39	3012	Angew Chem, Int Ed	HCAPLUS
Gierasch, T				Manuscript submitted	
Gierasch, T	2000	2	3999	Org Lett	HCAPLUS
Gordon, E	1988	31	2199	J Med Chem	HCAPLUS
Harrison, B	2002	124	13352	J Am Chem Soc	HCAPLUS
Harrison, B	2001	3	2157	Org Lett	HCAPLUS
Law, P	1999	51	440	Biopolymers	HCAPLUS
Michielin, O	2002	124	11131	J Am Chem Soc	HCAPLUS
Nicolaou, K	2000	122	9954	J Am Chem Soc	HCAPLUS
Pasternak, G	2001	68	2213	Life Sci	HCAPLUS
Pasternak, G	1990	6	1	Mod Methods Pharmaco	HCAPLUS
Pelish, H	2001	123	6740	J Am Chem Soc	HCAPLUS
Scholl, M	1999	1	953	Org Lett	HCAPLUS
Schreiber, S	2000	287	1964	Science	HCAPLUS
Standifer, K	1997	9	237	Cell Signalling	HCAPLUS
Stockwell, B	2000	1	116	Nat Rev Genet	HCAPLUS
Tan, D	1998	120	8565	J Am Chem Soc	HCAPLUS
Zadina, J	1999	897	136	Ann N Y Acad Sci	HCAPLUS
Zadina, J	1997	386	499	Nature	HCAPLUS

L21 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:72698 HCAPLUS Full-text
DN 138:271935
TI 2,6-Dimethyltyrosine Analogues of a Stereodiversified Ligand Library: Highly Potent, Selective, Non-Peptidic μ Opioid Receptor Agonists
AU **Harrison, Bryce A.**; Pasternak, Gavril W.; **Verdine, Gregory L.**
CS Department of Chemistry and Chemical Biology, **Harvard** University, Cambridge, MA, 02138, USA
SO Journal of Medicinal Chemistry (2003), 46(5), 677-680
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 138:271935
GI



I

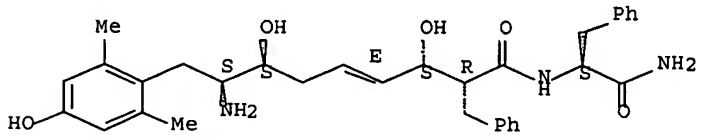
AB The authors report the synthesis and bioactivity of enediol-based 2,6-dimethyltyrosine analogs I (X = NH, R = CONH2; X = NH, R = H; X = NH, R = CH2OH; X = O, R = CONH2; X = O, R = H; X = O, R = CH2OH) towards μ-opioid receptor. For I (X = NH, R = CONH2; X = NH, R = H), five stereoisomers of each compound were synthesized and their bioactivity evaluated, discovering certain stereoisomers with unexpected potency, selectivity, and efficacy.

IT **503186-38-7P 503186-39-8P 503186-40-1P**
503186-41-2P 503186-42-3P 503186-43-4P
503186-44-5P 503186-45-6P 503186-46-7P
503186-47-8P 503186-48-9P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(asym. preparation of enediol-based nonpeptidic analogs of dimethyltyrosine and their evaluation as μ-opioid receptor agonists)

IT **503186-38-7P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(asym. preparation of enediol-based nonpeptidic analogs of dimethyltyrosine and their evaluation as μ-opioid receptor agonists)

RN 503186-38-7 HCAPLUS
CN Benzenepropanamide, α-[(1S,2E,5S,6S)-6-amino-1,5-dihydroxy-7-(4-hydroxy-2,6-dimethylphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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Adamson, J	1991	56	3447	J Org Chem	HCAPLUS
Balboni, G	2002	45	713	J Med Chem	HCAPLUS
Blackwell, H	2000	122	58	J Am Chem Soc	HCAPLUS
Chandrakumar, N	1992	35	223	J Med Chem	HCAPLUS
Chandrakumar, N	1992	35	2928	J Med Chem	HCAPLUS
Furstner, A	2000	39	3012	Angew Chem, Int Ed	HCAPLUS
Gierasch, T	2000	2	3999	Org Lett	HCAPLUS
Hansen, D	1992	35	684	J Med Chem	HCAPLUS
Harrison, B	2002	124	13352	J Am Chem Soc	HCAPLUS
Harrison, B	2001	3	2157	Org Lett	HCAPLUS
Michielin, O	2002	124	11131	J Am Chem Soc	HCAPLUS
Nicolaou, K	2000	122	9954	J Am Chem Soc	HCAPLUS
Pasternak, G	1990	6	1	Mod Methods Pharmaco	HCAPLUS
Pelish, H	2001	123	6740	J Am Chem Soc	HCAPLUS
Pitzele, B	1994	37	888	J Med Chem	HCAPLUS
Salvadori, S	1999	42	5010	J Med Chem	HCAPLUS
Schiller, P	2000	35	895	Eur J Med Chem	HCAPLUS
Schiller, P	1999	42	3520	J Med Chem	HCAPLUS
Scholl, M	1999	1	953	Org Lett	HCAPLUS
Schreiber, S	2000	287	1964	Science	HCAPLUS
Stockwell, B	2000	1	116	Nat Rev Genet	HCAPLUS
Tan, D	1998	120	8565	J Am Chem Soc	HCAPLUS
Zadina, J	1999	897	136	Ann N Y Acad Sci	HCAPLUS
Zadina, J	1997	386	499	Nature	HCAPLUS

L21 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:808520 HCAPLUS Full-text
DN 138:55660
TI High-Affinity Mu Opioid Receptor Ligands Discovered by the Screening of an Exhaustively Stereodiversified Library of 1,5-Enediols
AU **Harrison, Bryce A.**; **Gierasch, Tiffany Malinky**; Neilan, Claire; Pasternak, Gavril W.; **Verdine, Gregory L.**
CS Department of Chemistry and Chemical Biology, **Harvard** University, Cambridge, MA, 02138, USA
SO Journal of the American Chemical Society (2002), 124(45), 13352-13353
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 138:55660
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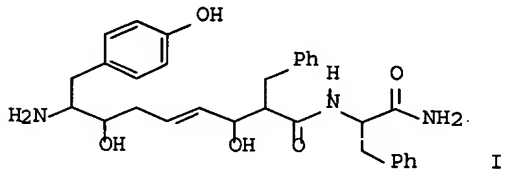

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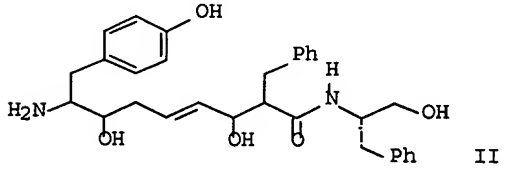

II

AB A stereodiversified library of all 16 stereoisomers of 1,5-enediol I was synthesized, and these compds. were screened for mu opioid receptor (MOR) binding. The stereochem. configuration of I strongly impacted the binding affinity, and (S,S,S,R)-I exhibited a Ki of 8.8 nM for MOR, comparable to that of endomorphin-2 (Ki = 1.2 nM). Moreover, compds. I exhibited 5-86-fold selectivity for MOR over delta opioid receptor (DOR) and 16-150-fold selectivity for MOR over kappa opioid receptor (KOR). Addnl., analogs of I were synthesized which showed that the trans configuration of the olefin was important for receptor binding but modifications of the C-terminal amino acid were well tolerated. Of these analogs, tetraols II are noteworthy because they retain only one of the amide bonds present in endomorphin-2, but bind MOR with an affinity of 10 nM and 110- and 600-fold selectivity for MOR over DOR and KOR. These results demonstrate the utility of stereochem. diversity in the discovery of bioactive small mols.

IT **479495-67-5P 479495-68-6P 479495-69-7P**
479495-70-0P 479495-71-1P 479495-72-2P
479495-73-3P 479495-74-4P 479495-75-5P
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479495-82-4P 479495-83-5P 479495-84-6P
479495-85-7P 479495-86-8P 479496-03-2P
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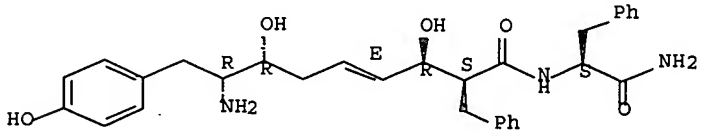
479496-17-8P 479496-18-9P 479496-19-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of amino(dihydroxy)nonenamides and derivs. as nonpeptidic high-affinity μ-opioid receptor ligands)

IT **479495-67-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of amino(dihydroxy)nonenamides and derivs. as nonpeptidic high-affinity μ-opioid receptor ligands)

RN 479495-67-5 HCAPLUS

CN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Annis, D	1998	37	1907	Angew Chem, Int Ed	HCAPLUS
Blackwell, H	2000	122	58	J Am Chem Soc	HCAPLUS
Bunin, B	1997	21	125	New J Chem	HCAPLUS
Cusack, N	1976	32	2157	Tetrahedron	HCAPLUS
Dooley, C	1999	51	379	Biopolymers	HCAPLUS
Furstner, A	2000	39	3012	Angew Chem, Int Ed	HCAPLUS
Gierasch, T	2000	2	3999	Org Lett	HCAPLUS
Harrison, B	2001	3	2157	Org Lett	HCAPLUS
Hruby, V	1999	51	391	Biopolymers	HCAPLUS
Kingsbury, C	1999	3	497	Curr Org Chem	HCAPLUS
Lacombe, P	1998	39	6785	Tetrahedron Lett	HCAPLUS
Mitchison, T	1994	1	3	Chem Biol	HCAPLUS
Nicolaou, K	2000	122	9954	J Am Chem Soc	HCAPLUS

Pasternak, G	2001	68	2213	Life Sci	HCAPLUS
Pasternak, G	1990	6	1	Mod Methods Pharmaco	HCAPLUS
Paterson, I	1999		1003	J Chem Soc, Perkins	HCAPLUS
Paterson, I	1992	33	797	Tetrahedron Lett	HCAPLUS
Scholl, M	1999	1	953	Org Lett	HCAPLUS
Schreiber, S	1998	6	1127	Bioorg Med Chem	HCAPLUS
Schreiber, S	2000	287	1964	Science	HCAPLUS
Standifer, K	1997	9	237	Cell Signalling	HCAPLUS
Stockwell, B	2000	1	116	Nat Rev Genet	HCAPLUS
Tan, D	1998	120	8565	J Am Chem Soc	HCAPLUS
Zadina, J	1999	897	136	Ann N Y Acad Sci	HCAPLUS
Zadina, J	1997	386	499	Nature	HCAPLUS

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L22 ANSWER 1 OF 1 USPATFULL on STN
AN 2004:321570 USPATFULL Full-text
TI Mu opioid receptor ligands: methods of use and synthesis
IN Harrison, Bryce A., Hamilton, NJ, UNITED STATES
Gierasch, Tiffany M., Bryn Mawr, PA, UNITED STATES
Verdine, Gregory L., Newton, MA, UNITED STATES
Shi, Zhangjie, Chicago, IL, UNITED STATES
PI US2004254225 A1 20041216
AI 2003US-0683756 A1 20031010 (10)
PRAI 2002US-417925P 20021011 (60)
2003US-443428P 20030129 (60)
DT Utility
FS APPLICATION
LREP EDWARDS & ANGELL, LLP, P.O. BOX 55874, BOSTON, MA, 02205
CLMN Number of Claims: 38
ECL Exemplary Claim: 1
DRWN 4 Drawing Page(s)
LN.CNT 3735
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds and compositions including those compounds, as well as methods of using and making the compounds are herein described. The compounds are useful in therapeutic applications, including modulation of disease or disease symptoms in a subject (e.g., mammal, human, dog, cat, horse). The compounds are useful as modulators of the mu opioid receptor (MOR) through their binding affinity with that receptor.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 479495-67-5P 479495-68-6P 479495-69-7P
479495-70-0P 479495-71-1P 479495-72-2P
479495-73-3P 479495-74-4P 479495-75-5P
479495-76-6P 479495-77-7P 479495-78-8P
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479496-12-3P 479496-13-4P 479496-14-5P
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507276-69-9P 507276-71-3P
(preparation of peptidomimetic μ-opioid receptor ligands)

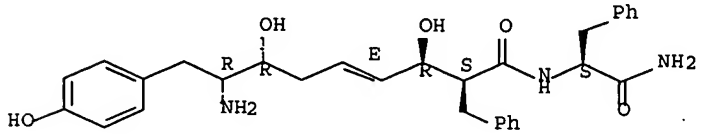
IT 680187-48-8DP, resin-bound 680187-49-9DP, resin-bound
680187-50-2DP, resin-bound 680187-51-3DP, resin-bound
(preparation of peptidomimetic μ-opioid receptor ligands)

IT 479495-67-5P
(preparation of peptidomimetic μ-opioid receptor ligands)

RN 479495-67-5 USPATFULL

CN Benzenepropanamide, α-[(1R,2E,5R,6R)-6-amino-1,5-dihydroxy-7-(4-hydroxyphenyl)-2-heptenyl]-N-[(1S)-2-amino-2-oxo-1-(phenylmethyl)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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L9 0 L8 SAM SUB=L7
L10 63 L7 AND L3
L11 0 L8 FULL SUB=L7

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E GIERASCH T/AU
L15 6 E4-5
E VERDINE G/AU
L16 195 E4-7
E SHI Z/AU
L17 395 E3-24

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